Report on Convergence and Refinement of the Wang-Landau Algorithm

Abdulkhaligov Rashad
Faculty of Informatics
Eötvös Loránd University
H-1053 Budapest, Egyetem tér 1-3
vs7vsr@inf.elte.hu

1 Ising model

The Ising model is a mathematical model that describes the behavior of interacting spins in a lattice, and it is a fundamental model in statistical mechanics. The model consists of a set of discrete variables, i, representing magnetic dipole moments of atomic "spins" that can be in one of two states (+1 or 1). These spins are located at the nodes of a lattice, allowing each spin to interact with its neighbors. The Hamiltonian of the Ising model can be written as:

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - \mu \sum_{i=1}^{N} B_i \sigma_i \tag{1}$$

where J is the exchange coupling constant, is the magnetic moment, B is the magnetic field, and N is the total number of spins in the lattice. The first term in the Hamiltonian represents the energy due to the interaction between neighboring spins, where the sum is taken over all pairs of neighboring spins, denoted by $\langle$i,j$\rangle$. The second term in the Hamiltonian represents the energy due to the interaction of each spin with the external magnetic field.

Ising models are often examined without an external field interacting with the lattice, that is, h = 0 for all i in the lattice Λ. Using this simplification, the Hamiltonian becomes

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{2}$$

The Ising model is a simple yet powerful tool to study phase transitions in magnetic materials. At low temperatures, the spins tend to align and the system exhibits ferromagnetism. At high temperatures, the spins are disordered and the system exhibits paramagnetism. The critical temperature at which the system undergoes a phase transition is known as the Curie temperature. The behavior of the system near the critical temperature can be described by mean-field theory or by renormalization group theory. The Ising model has been widely used to study critical phenomena in various physical systems, such as magnets, alloys, and superfluids.

2 Wang Landau Method

The Wang-Landau algorithm is a Monte Carlo simulation technique used to compute the density of states of a given system, which is an essential quantity in statistical mechanics. It was proposed by Fugao Wang and David P. Landau in 2001 [1] [2] [3] [4], and since then, it has become a popular method for studying various physical systems.

The algorithm works by gradually updating the density of states of a system in a way that ensures that all energy states are sampled equally. This is achieved by modifying the probability of accepting a trial move in a Monte Carlo simulation. At each iteration, the probability is multiplied by a weight factor that depends on the current estimate of the density of states. The algorithm continues until the density of states converges to a flat distribution.

Mathematically, the Wang-Landau algorithm can be expressed as follows:

Let E_i be the energy of the ith microstate of the system, and let $g(E_i)$ be the density of states at energy E_i. The goal of the algorithm is to estimate $g(E_i)$ for all possible values of E_i. At each iteration of the algorithm, a random microstate is selected, and a trial move is proposed. The move is accepted with probability

$$P_{accept} = \min\left[1, \frac{g(E_{i-1})}{g(E_i)}\right] \tag{3}$$

where E_{i-1} and E_i are the energies of the current and proposed microstates, respectively. The acceptance probability is modified by a weight factor $f(E_i)$, which is updated at each iteration as follows:

$$f(E_i) = f(E_i) \times \frac{1}{f_{max}} \tag{4}$$

where f_{max} is the maximum value of $f(E_i)$ obtained so far. The weight factor ensures that the acceptance probability eventually becomes uniform for all energy states.

The algorithm terminates when the density of states converges to a flat distribution within a given tolerance. Once the density of states has been estimated, various thermodynamic quantities such as the free energy and specific heat can be calculated.

Wang-Landau method is a powerful and efficient algorithm for calculating the density of states in statistical mechanics. Its ability to explore the energy landscape of complex systems makes it a valuable tool for studying a wide range of phenomena, including phase transitions, energy barriers, and the behavior of disordered systems.

The algorithm's ability to accurately reproduce the exact density of states in simple systems, such as the Ising model, demonstrates its potential for use in more complex systems where analytical solutions are not available.

[2]

Algorithm 1 Wang-Landau Algorithm

Initial configuration S_0, modification factor f_0, tolerance ϵ Density of states $f(E)$

1. Set $g(E) \leftarrow 1$ for all energies E;

2. Randomly flip spin with probability $p(E_1 \rightarrow E_2) = \min\left[1, \frac{g(E_1)}{g(E_2)}\right]$;

3. Set $g(E) \rightarrow g(E) \cdot f, H(E) = H(E) + 1$;

4. Continue until the histogram is flat, decrease f, and reset the histogram to $H(E) = 0$;

5. Repeat steps 2 - 4 until f is very small;

3 Convergence and Refinement of the Wang-Landau Algorithm

We analyzed the Monte Carlo time dependence of ΔH_k at each iteration using the Wang-Landau method, where the subscript k denotes the kth iteration. Simulations were conducted on an Ising model with a system size of 8.

Figure 1 displays the time dependence of ΔH_k for various values of $\log(f)$, where $\log(f) = 10^{-2}, 10^{-3}, 10^{-4}$, and 10^{-5} from left to right, top to bottom, respectively. We used a sequence

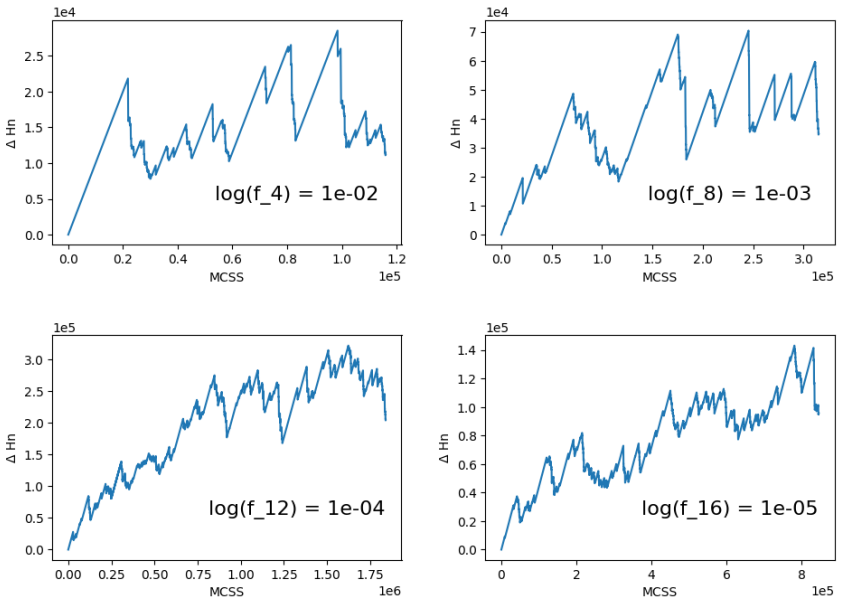

Figure 1: Caption of the figure.

of correction factors $\log(f_{k+1}) = \log(f_k)/1.78$ with $\log(f_1) = 0.1$. This sequence was chosen so that $\log(f_{k+4}) = \log(f_k)/10$. These graphs were obtained by implementing the Wang-Landau algorithm on an 8x8 ferromagnetic Ising model with numerical values averaged over 32 independent simulations. The horizontal axis of Figure 1 represents the Monte Carlo steps per spin measured from the time when we decrease $\log(f)$. ΔH_k increases initially and eventually saturates, and for smaller values of $\log(f)$, the saturation values are larger, and the number of Monte Carlo steps required to reach saturation is greater.

$$\eta_n = \sum_E [\log \tilde{g}_\infty(E) - \log \tilde{g}_n(E)] = \sum_{k=n+1}^{\infty} \Delta H_k \log(f_k) \tag{5}$$

Since the error term[5] given by Equation (5) depends only on ΔH_k, any computational effort after ΔH_k becomes saturated does not enhance the accuracy of the final density of states $g_n(E)$. However, stopping the random walk before ΔH_k becomes saturated would make the simulation less efficient since insufficient statistics are accumulated in the kth iteration, and much more statistics would have to be collected with smaller $\log(f)$ values for subsequent iterations. An optimal algorithm is to terminate the simulation as soon as ΔH_k reaches saturation.

References

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